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Analysis of residual acceleration effects on transport and segregation during directional solidification of tin-bismuth in the MEPHISTO furnace facility

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Objectives

The object of this work, started in March of 1995, is to approach the problem of determining the transport conditions (and effects of residual acceleration) during the plane-front directional solidification of a tin-bismuth alloy under low gravity conditions. The work involves using a combination of 2- and 3-D numerical models, scaling analyses, 1D models and the results of ground-based and low-gravity experiments. The experiments conducted in the MEPHISTO furnace facility during the USMP-3 spaceflight which took place earlier this year (February 22 through March 6, 1996). This experiment represents an unprecedented opportunity to make a quantitative correlation between residual accelerations and the response of an actual experimental solidification system

Introduction

Real-time Seebeck voltage variations across a Sn-Bi melt during directional solidification in MEPHISTO on USMP-1 showed a distinct variation which can be correlated with thruster firings. The Seebeck voltage measurement is related to the response of the instantaneous average melt composition at the melt-solid interface. This permitted a direct comparison of numerical simulations (and acceleration data) with the Seebeck signals obtained on USMP-1. Motivated by the results of the comparison we used numerical simulations to predict the response of the Seebeck signal to composition changes at the interface caused by convective disturbances produced by thruster firings of various magnitudes and durations. These simulations were carried out for different solidification rates. The results of the simulations were used to plan a subset of the USMP-3 MEPHISTO experiments dedicated to the evaluation of g-jitter effects. There were several differences between the USMP-3 experiments as compared to USMP-1. Firstly, a more concentrated alloy was solidified on USMP-3, and, secondly, Primary Reaction Control System (PRCS) thruster burns were requested at particular times during four separate growth runs. This allowed us to monitor the Seebeck signal response under well-characterized growth conditions. This allowed for quantification of the effects of "g-jitter" on convective-diffusive transport in the melt through the real-time changes in average interfacial composition obtained from the Seebeck measurement. In addition, guided by SAMS acceleration data, we carried out simulations during the experiment in order to obtain a better comparison of predicted responses with the actual Seebeck signal. Preliminary results are described below.

Approach

Our approach relied primarily on the use of numerical models to simulate the response of transport behavior in the directionally solidifying tin-bismuth to particular types of g-jitter. In particular, since specific accelerations (corresponding to unidirectional acceleration of a given fixed magnitude, orientation and duration) were requested at specific times during the experiments, the modeling focused primarily on "impulse"-type acceleration.

A sketch of the experiment set-up is shown in Fig. 1. There are two furnaces, one is fixed, the other is translated through a temperature gradient. The applied temperature profile shown in Fig. 1 leads to a central cylindrical melt volume bounded by a moving and a stationary (or reference) solid-liquid interface. The melt composition at the moving and the stationary reference interfaces is not the same. For Sn-Bi there is a dependence of melting temperature on concentration. Thus, it follows that the melting temperature at the two interfaces will not be the same. The Seebeck effect gives rise to a small but measurable voltage difference between these two interfaces. Measurement of this voltage difference

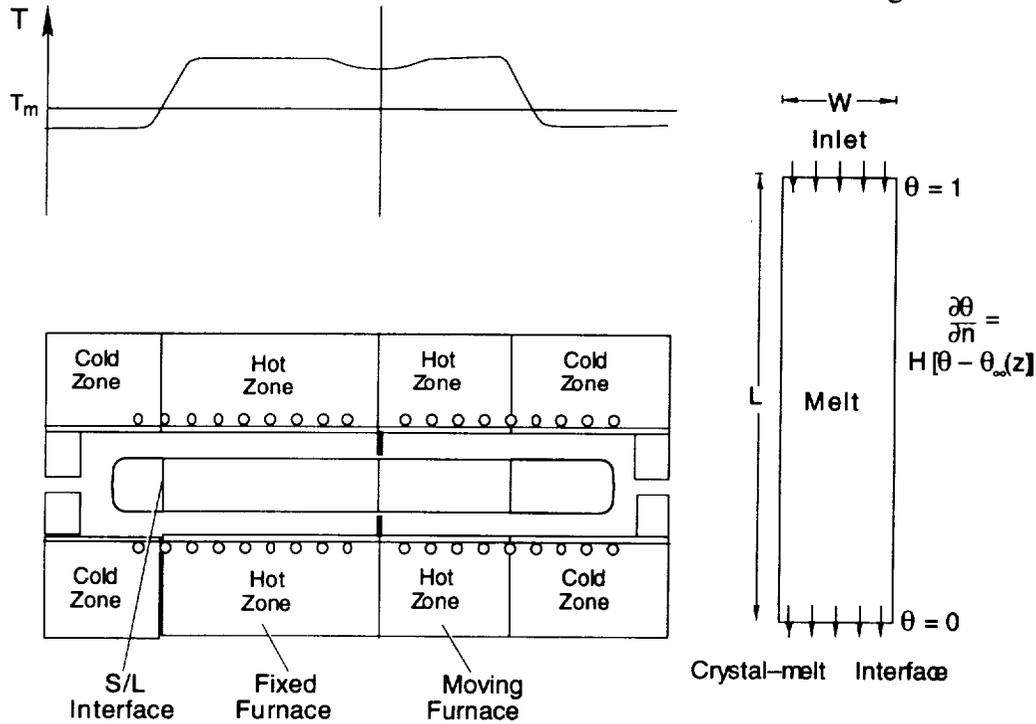


Fig. 1 The MEPHISTO set-up (bottom-left), temperature profile (top left) and computational model (right). T_m denotes the melting temperature.

allows the determination of the average temperature and, thus, the average composition of at the growing interface. The MEPHISTO set-up and the Seebeck measurements are discussed in more detail in [1].

The basic model system used for the simulations has been described elsewhere [2,3]. The essential features are outlined below. Solidification takes place as the ampoule is translated along a temperature gradient. For this model system, translation of the ampoule is simulated by supplying a doped melt of bulk composition c_∞ at a constant velocity V_g at the top of the computational space (inlet), and withdrawing a solid of composition $c_s = c_s(x,t)$ from the bottom. The crystal-melt interface is located at a distance L from the inlet; the width of the ampoule is W . The temperature at the interface is taken to be T_m , the melting temperature of the crystal, while the upper boundary is held at a higher temperature T_h . The ampoule wall temperatures are prescribed according to the particular situation to be modeled. Since we wish to confine our attention to compositional nonuniformities caused by buoyancy-driven convection, rather than variations resulting from non-planar crystal-melt interfaces, the interface is held flat. We expect that, given the large ($175 - 195 \text{ K cm}^{-1}$, temperature gradient) that changes in melting temperature due to compositional non-uniformity will not lead to significant changes in interface shape due to interfacial compositional inhomogeneity. In addition, because of the melt's low Prandtl

number together with the low magnitude accelerations, convection does not lead to significant deviations of the temperature from the conductive state and, thus, changes in the interface shape due to changes in the thermal field will be negligible. The governing equations governing coupled convective-diffusive heat mass and species transfer in the melt are taken to be the Oberbeck-Boussinesq equations which are solved using a Chebyshev spectral method.

In an actual experiment, owing to the finite length of the ampoule, there is a gradual decrease in length of the melt zone during growth. In this model, transient effects related to the change in melt length are ignored. Since the MEPHISTO experiments involves melt lengths that are far in excess of the ampoule diameter, this does not preclude us from calculating the compositional transient. That is, we can start the calculations by solidifying from an initially uniform composition melt. Our results, when compared to experiment, reveal that this assumption is justified. The thruster firings are simulated using impulsive accelerations which are introduced through a time-dependent body-force term g . During the first year of this grant we calculated the response of the system to impulsive accelerations of various magnitudes and durations. Preliminary results are described in [4].

During the recent USMP-3 experiments the first quantitative experimental results concerning the effects of microgravity disturbances on the directional solidification. Comparison of the real-time (raw, uncorrected) Seebeck signals with the predicted Seebeck signal calculated from the evolution of the simulated composition profiles showed excellent agreement. Selected examples of the results obtained during the USMP-3 mission will be discussed in more detail the workshop.

Ongoing work

Detailed analysis of the experimental results (by the Grenoble group) is currently in progress and we are coordinating our ongoing work accordingly.

In addition to the work specifically related to the USMP-3 experiment, we have undertaken an extensive analysis of the effects of vibration (coupled with steady acceleration) on convection, heat and mass transport. For the case of thermovibrational convection of a Boussinesq fluid contained in a closed differentially heated rigid-walled 2D cavity we have found that chaotic flow responses occur at high vibration amplitudes. In the absence of vibration a steady (intermediate Rayleigh number, Ra) buoyancy-driven flow occurs. The simulations were undertaken by direct solution of the Navier-Stokes-Boussinesq equations using a pseudo-spectral Chebyshev collocation method. Four basic regimes are recognized: quasi-static, oscillatory, asymptotic and a fourth regime, which appears for certain values of the vibrational Rayleigh number as a wedge-shaped region which separates the oscillatory and asymptotic regimes. This region is characterized by two-periodic, sub-harmonic cascades and chaotic behavior and represents that region of parameter space where the vibrating fluid behaves as an unstable dissipative oscillator. Here the vibration of the cavity results in a parametrically excited motion that exhibits a variety of nonlinear behavior depending on the relationship between the forcing frequency and the resonant frequency of the fluid system. At twice the Brünt-Väisälä frequency of the system a continuous transition from simple periodic oscillations to a subharmonic cascade toward chaotic responses is observed as the vibration amplitude is increased. In the absence of vibrational motion, chaotic motion would be expected to occur only at very large values of the Rayleigh number. Thus, it appears that simple translational low frequency oscillations of the cavity can lead to transitions to chaos at relative low values of Ra . A brief overview of these results will also be presented at the workshop.

References

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